

MODEL OF 2 LAYER SEDIMENT CAP, DESCRIPTION AND PARAMETERS

Version - 2 Layer Analytical Model v.1.18 and Active Cap Layer Model v 4.1

This Excel spreadsheet model contains three worksheets

1. A two layer (bioturbation and chemical isolation layer) analytical model of steady state cap performance
2. A one layer (chemical isolation layer) analytical model of transient cap performance
3. A sensitivity analysis of the two layer steady state model

The steady state analytical model evaluates the long time behavior of a cap, after both the biologically active layer and the underlying cap layer are influenced by contaminant migration from below. It estimates the maximum concentration or flux that can ever be expected from a cap assuming that the underlying concentration is constant. The model implemented in the spreadsheet is a two layer steady state model which predicts concentrations and fluxes in a chemical isolation layer or in the near surface biologically active zone or bioturbation layer. The model is described in detail in Lampert and Reible ¹. The transient model is designed to describe chemical migration in the chemical isolation layer of a cap only. The model is set up to stop calculations at a point in time when the concentration in the bioturbation layer begins to be significant (although the end time of the transient calculation can be overwritten, the user should do so with caution because the transient model does not account for the faster transport and degradation processes in the biologically active zone). The sensitivity analysis worksheet is designed to allow easy adjustment of model parameters to look at a large number of conditions quickly.

The active cap layer model v 4 is identical to the conventional model (v. 1.18) except that it treats the lower layer as an amended cap layer (e.g. amended with activated carbon or organoclay with assumed linear partitioning) and the upper layer is a conventional sand cap layer. Since both layers are part of the cap, the active cap layer model does not evaluate a bioturbation layer. Previous versions of the active layer model (before v 4) used a different approach to estimate the active layer thickness and the approximations used were valid in only a narrow range of conditions. Because many people were using the model outside of that range of conditions, it was deemed appropriate to eliminate that model and replace it with the v. 4. The modeling remains approximate although the primary limitation of v4 is the use of linear sorption (which is often not a valid assumption for activated carbon, in particular). For

¹ *Lampert, D.J. and Reible, D.D. 2008. "An Analytical Modeling Approach for Evaluation of Capping of Contaminated Sediments," Soil & Sediment Contamination, (under review)."

full simulation of such cases, a numerical model such as CAPSIM 2 should be employed. The latter model is also available from Danny Reible at reible@mail.utexas.edu.

Model parameters and their definitions are shown below. Although the parameters are used to define both the steady state and transient model, note that many are not applicable in the transient model since it describes migration in only a single capping isolation layer (as modified by the effective thickness of an active cap layer). Parameters shown in the spreadsheet in blue are normal model inputs that the user is free to change as needed. Parameters shown in yellow are parameter estimates that employ the user supplied inputs and represent best estimates based upon the author's experience. These parameters can be changed but the reader is cautioned in doing so. Parameters shown in red are integral to the model and these values should not normally be changed.

Values in blue – change as appropriate for your site

Values in yellow – change if you have a more appropriate parameter estimation approach or a measured value

Values in red – should not normally be changed in that they are integral to the model

Contaminant Properties

Contaminant – Identification of contaminant for easy reference

Octanol-water Partition Coefficient, log K_{ow} – Tabulated K_{ow} values are used to estimate contaminant hydrophobicity and to calculate other parameters including organic carbon based partition coefficient and the dissolved organic carbon based partition coefficient.

Water Diffusivity, D_w – diffusivity of the pure contaminant in water, cm^2/sec

Cap Decay Rate (porewater basis), λ_1 – contaminant degradation rate in cap interstitial waters, yr^{-1}

Bioturbation Layer Decay Rate (porewater basis), λ_2 – contaminant degradation rate in interstitial water of surficial biologically active layer in yr^{-1}

Sediment Layer Properties (Active Layer Model- Sediment/Conventional Cap Properties)

Contaminant Pore Water Concentration, C_θ – Interstitial concentration in the near surface layer of the underlying sediment, $\mu\text{g/L}$

Biological Active Zone fraction organic carbon, $(f_{oc})_{bio}$ (Active Layer model – Conventional cap layer fraction organic carbon) Surficial layer organic carbon content (as a fraction of sediment dry weight), assumed to apply to both the underlying sediment before capping and the surficial cap layer at steady state (after deposition of new sediment).

Colloidal Organic Carbon Concentration, ρ_{DOC} –dissolved organic carbon in sediment and cap interstitial waters, mg/L

Darcy Velocity, V – volume of upwelling water discharging into overlying water body per unit surface area per time, $\text{cm}^3/(\text{cm}^2 \cdot \text{yr})$. V is forced ≥ 0 , that is, losing bodies of water (downward velocity) are estimated conservatively as diffusion only

Depositional Velocity, V_{dep} – rate of deposition of new sediment in cm/yr . The deposition velocity is used to estimate an effective Darcy velocity using the sorption characteristics of the chemical isolation layer. Note that a large deposition velocity can give rise to an ever increasing cap thickness that will give large negative effective velocities. The calculated effective Darcy velocity is limited to that which would offset diffusion to avoid physically unrealistic solutions (i.e. total upward migration cannot be less than 0)

Bioturbation Layer Thickness, h_{bio} – thickness, in cm , of the biologically active layer that will develop at the surface of the cap. Figure 1 shows the probability distribution for this parameter in freshwater (median=4.8 cm) and estuarine systems (median=7.9 cm).

Pore Water Biodiffusion Coefficient, D_{bio}^{PW} – effective diffusion coefficient in biologically active layer based on interstitial water, cm^2/yr . There is very little guidance for this parameter although measurements have shown 10^{-3} - 10^{-5} cm^2/s as reasonable estimates. Since the parameter also characterizes organism behavior, using a multiple of the particle diffusion coefficient below (e.g. $100 \times D_{bio}^P$) might be a reasonable estimation method. Note that although the numerical value of this parameter may be larger than D_{bio}^P , particle biodiffusion is typically more important due to contaminant sorption on the particles.

Particle Biodiffusion Coefficient, D_{bio}^P – effective particle diffusion coefficient in biological active layer, cm^2/yr . Figure 2 shows the probability distribution for this parameter in freshwater (median = 3.3×10^{-8} cm^2/sec = $1.06 \text{ cm}^2/\text{yr}$) and estuarine systems (median= 3×10^{-7} cm^2/sec = $9.4 \text{ cm}^2/\text{yr}$)

In the active layer model, the preceding three parameters are replaced with the conventional cap placed thickness, consolidation depth, a calculated conventional cap layer thickness (in red), a cap materials type, a particle density and calculated effective diffusion coefficient (in yellow).

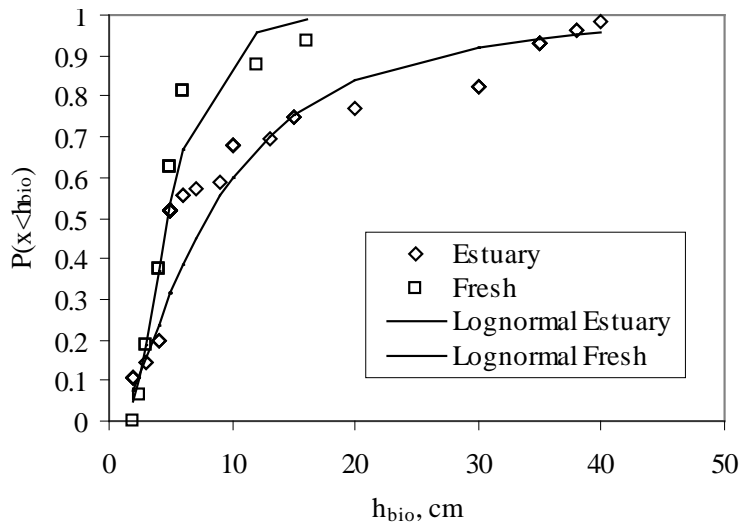


Figure 1- Distribution of measurements of h_{bio} (adapted from Thoms et al., 1995)

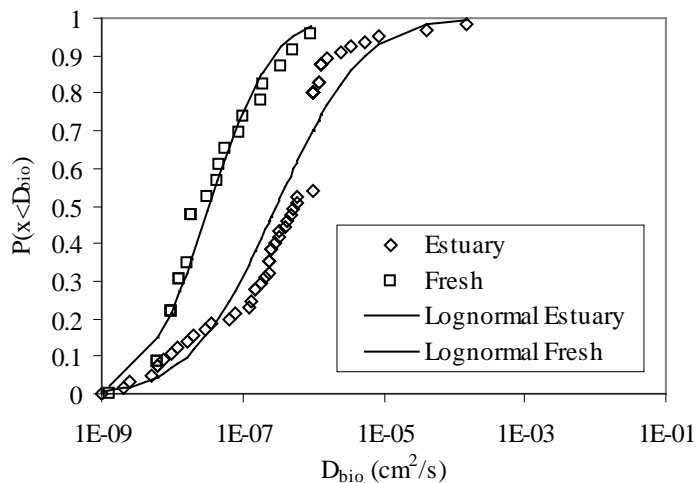


Figure 2 -Distribution of measurements of D_{bio} (adapted from Thoms et al., 1995)

Cap Properties (Active Cap Properties in the Active Cap model)

Conventional Cap placed depth (total cap placed depth in active layer model)– The depth of placed sand or other conventional cap material, in cm. The effective depth will be less due to bioturbation or consolidation

Cap Materials – If the cap is constructed of sand or similar material, a G (granular) should be entered here, whereas if it is constructed of silt or clay, C should be entered for a consolidated material. Two different models of estimating the effective diffusion coefficient are employed for these two types of materials.

Cap consolidation depth – Depth that the cap consolidates (typically small for a sandy cap), in cm. This does not include the consolidation of the underlying sediment.

Underlying sediment consolidation due to cap placement – Underlying sediment consolidation, in cm. This indicates the total volume of porewater expressed into the cap layer. The migration of a contaminant

expressed with this porewater may be considerably less than the total consolidation due to sorption-related retardation in the cap material.

Porosity, ε – Void fraction in conventional cap material

Particle Density, ρ_P – Cap amendment density, in g/cm³ (note- in the active cap model this does not have to be total density but only the density of the active material in the cap)

Fraction organic carbon, $(f_{oc})_{eff}$ – Fraction organic carbon in conventional cap material

In the active cap layer model, this parameter is replaced with an effective K_d (assumed constant for linear partitioning) in the active layer

Depth of Specific Interest below cap-water interface, z – If performance (as indicated by porewater or bulk solid phase concentration) at a particular distance below the cap surface is desired, this depth can be entered here, in cm.

Fraction organic carbon at depth of interest, $f_{oc}(z)$ – Fraction organic carbon at the depth of interest which is used to estimate the bulk solid phase concentration from the porewater concentration with the relationship $W = K_{oc} f_{oc} C_{pw}$. Use of this parameter allows one to use the fraction organic carbon of either the biologically active zone or the underlying cap layer if the depth of interest is set at the bottom of the biologically active zone.

Steady State Equivalent Cap thickness, h_{cap} – Calculated effective thickness of overall cap for steady state calculations including both sand cap and active cap layer, in cm

Transient Equivalent cap thickness, h_{equiv} - Calculated effective thickness of overall cap for transient calculations including both sand cap and active cap layer, in cm

Effective cap partition coefficient – Calculated effective cap partition coefficient in L/kg

Commonly Used Parameter Estimates (can be changed)

Organic carbon based Partition Coefficient, $\log K_{oc}$ – This quantity is calculated from the formula $0.903 \log K_{ow} + 0.094$ (Baker²). The K_{oc} is used to estimate the sediment-water partition coefficient through the formula $K_d = K_{oc} f_{oc}$ where f_{oc} is the fraction organic carbon of the layer of interest. Note that inorganic contaminants can be simulated by including an effective $\log K_d$ as the $\log K_{oc}$ entry and choosing $f_{oc} = 1$

Colloidal Organic Carbon Partition Coefficient, $\log K_{doc}$ – dissolved organic matter can increase the mobile fraction of contaminant. For PAHs, Burkard³ has suggested $\log K_{doc} = \log K_{ow} - 0.58$ where K_{ow} is the tabulated octanol-water partition coefficient

Boundary Layer Mass Transfer Coefficient, k_{bl} – benthic boundary layer mass transfer coefficient, cm/yr. A typical value is 1 cm/hr. A useful model of this parameter is

² Baker, J.R., Mihelcic, J.R., Luehrs, D.C., and Hickey, J.P. 1997. "Evaluation of Estimation Methods for Organic Carbon Normalized Sorption Coefficients," Water Environment Federation, 69(2):136-145.

³ Burkhard LP. 2000. Estimating dissolved organic carbon partition coefficients for nonionic organic chemicals. Environ Sci Technol 34:4663-4668.

$$k_{bl} = \frac{v_w^{1/2} u_*^{1/2}}{Sc^{2/3} y_0^{1/2}}$$

Where v_w is the kinematic viscosity of water ($\sim 0.01 \text{ cm}^2/\text{sec}$), u_* is the friction velocity characterizing the shear stress at the sediment-water interface (typically, 1-5 cm/sec), y_0 is the hydrodynamic roughness of the sediment-water interface (typically 1-10 cm) and Sc is the Schmidt number, the ratio of kinematic viscosity of water to the molecular diffusion coefficient of the contaminant in water (of the order of 1000 for most contaminants in water).

Dispersivity, α - Dispersion is characterized by αU where U is the Darcy velocity. α is the order of the length scale of heterogeneities in the cap. In this version we employ a conservative estimate of dispersivity of 5% of the cap thickness. The Neuman⁴ groundwater model of $\alpha = 1.69(h_{\text{cap}}(\text{in m}))^{1.53}$ is employed except that α is not allowed to be less than 1 cm. Note that this is one of the most uncertain parameters in the simulation although it normally has little influence unless advection is strong.

Diffusion coefficient, D_1 – Diffusivity in cap layer is modeled as per Millington and Quirk⁵ if granular (sand, gravel) or Boudreau⁶ if consolidated sediment.

Millington and Quirk
$$D_{diff} = \varepsilon_1^{4/3} D_w$$

Boudreau
$$D_{diff} = \frac{\varepsilon_1 D_w}{1 - \ln \varepsilon_1^2}$$

Output-Steady State Model (Contents of these cells should not be changed)

Pore Water Concentration at Depth, $C(z)$ – Model calculated steady state porewater concentration in porewater at the specific depth of interest, in $\mu\text{g/L}$

Solid Concentration at Depth of Interest, $W(z)$ – Model calculated steady state bulk solid phase concentration in $\mu\text{g/kg}$

Average Bioturbation Layer Loading, $(W_{bio})_{avg}$ – Model calculated steady state average bulk solid phase concentration in the biologically active zone, in $\mu\text{g/kg}$

Flux to Overlying Water Column, J – Model calculated steady state flux to overlying water, $\mu\text{g/m}^2 \cdot \text{yr}$

Cap-Bioturbation Interface Concentration, C_{bio}/C_0 – Steady state porewater concentration at the cap bioturbation layer interface, in % of concentration in underlying sediment

Cap-Water Interface Concentration, C_{bl}/C_0 – Steady state porewater concentration at the cap water

⁴ Neuman, S.P. 1990. "Universal Scaling in Geologic Media," Water Resources Research, 26(8):1749-1758.

⁵ Millington, R.J., and Quirk, J.M. (1961) "Permeability of Porous Solids," Transactions of the Faraday Society, 57:1200-1207.

⁶ Boudreau, B. (1997) Diagenetic Models and Their Implementation: Modeling Transport Reactions in Aquatic Sediments. Springer-Verlag, New York.

interface, in % of concentration in underlying sediment

Average Bioturbation Concentration, (C_{bio})_{avg}/C₀ – Steady state average porewater concentration in the biologically active zone, in % of concentration in underlying sediment

Time to Containment Breakthrough, t_{adv/diff} – Time before significant concentrations are expected in the biological active zone. Also the time after which the transient analytical model (2nd tab) may begin to overestimate concentrations in the biologically active zone. It indicates the approximate time before the concentration and flux at the top of the chemical isolation layer is 1% of what it is in the sediments.

$$t_{adv/diff} \approx \frac{1}{1/t_{diff} + 1/t_{adv}} \approx \frac{1}{16D_1 / (R_1 h_{eff}^2) + U / (R_1 h_{eff})} \approx \frac{R_1 h_{eff}^2}{16D_1 + U h_{eff}}$$

Output - Transient Model (Transient Model Tab)

The model inputs summarized above are used to calculate key parameters for the transient model in the chemical isolation layer, i.e. the conventional sand layer as modified by the effective thickness of the active cap layer. These parameters include Peclet number (relating advection to diffusion, Dakhmkoher number (relating reaction to diffusion), and a parameter u which is affected by both diffusion and advection. The final parameter needed for the model is the simulation time. The time until significant concentrations are noted in the biologically active zone is t_{adv/diff}. This would normally be the simulation time although if the bioturbation rate in the biologically active zone (or migration rate through the conventional cap layer in the active layer model) is small or the concentration in that zone as predicted by the model at t_{adv/diff} is small, the simulation time can be extended to give estimates of concentration in the capping isolation layer over a longer period of time. This may be especially important with an active sorbing layer in that the concentrations in much of the capping isolation layer are very small and essentially uniform for long periods of time after some penetration of contaminants are noted in the biologically active layer. If a longer simulation time it can simply be entered in the identified cell. The output from the simulation is shown on a figure showing both transient curves at various times and the long-time steady state curve for comparison. The results are also shown as concentrations (as the ratio of concentration to underlying sediment concentration) as a function of depth (in cm) and time. Note that the output will provide increased resolution in the sorbing active cap layer as appropriate.

Sensitivity Model Tab

The final tab in the spreadsheet model is designed to conduct sensitivity analyses on the steady state model. The tab does not include capabilities for conducting sensitivity analyses on the transient model. On this tab, the model parameters can be varied as desired to evaluate the output variables, for example concentration at a specific point of interest or in the biologically active zone. Columns B and C should not be changed. Column B is tied to the parameter values on the steady state conditions tab while column C is tied to column B. Column C can be copied and the values pasted in any number of additional columns and then values of selected parameters changed in those columns to allow parameter values to be changed.